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Many-Building CFD Model Development

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Objectives: Modeling the transport and dispersion of airborne contaminants in an urban environment is challenging the capabilities of computational fluid dynamics (CFD) codes. The high resolution required to capture, for example, the recirculation regions that form on building surfaces or the channeling that occurs between buildings requires super-computer-type computational resources and high fidelity numerical schemes. These same building-induced flows obliges careful attention to the turbulent transport approximations inherent in CFD models. In addition, the many-building urban-scale problem resides somewhere between the traditional CFD modeling regime and the meteorological regime. Hence, to properly capture transport and dispersion phenomena on the urban scale requires that CFD codes incorporate meteorological physics. Finally, in order to provide timely insight into transport and dispersion problems, the numerics need to be made more efficient and algorithms must be developed to take full advantage of the parallel architecture of today's supercomputers. The LANL and LLNL effort in this area is focused on improving the CFD codes for specific applications in and benefit to the DOE CBNP program.

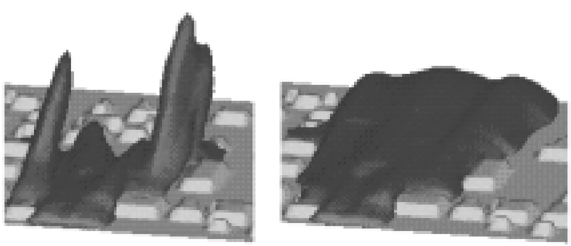

Figure 1. Daytime release through cluster of buildings demonstrating the impact of radiative heating on tracer dispersion. Radiative heating turned on (left) and turned off (right).

Recent Progress: *Surface Energy Budget*. A 1-D meteorological physics package has been incorporated into the HIGRAD model in order to simulate the effects of radiative heating in the atmosphere and ground surface. This package was adopted from a similar version presented by Smith and Kao (1996) and includes the treatment of shortwave and longwave radiation and surface fluxes of heat and moisture. Surface quantities are updated using a 5-layer surface model with specified albedo and emissivity for the surface, and specified heat capacity and thermal conductivity for each layer. Surface fluxes of heat and moisture are computed using Monin-Obhukov similarity theory. Reisner et al. (1998) showed that surface heating and building shading had a dramatic effect on transport and dispersion around clusters of buildings (Figure 1).

Numerical Fidelity. The atmosphere is inherently nonlinear, and the validity of the linear approximation used in implicit solvers is, for certain flow situations, somewhat questionable. To overcome the linear approximation, numerical modelers have recently combined two old techniques, Newton's method and Krylov solvers (e.g., conjugate gradient), in a clever manner such that nonlinear implicit equation sets can be solved.

Initial results using the Newton-Krylov approach suggest that neglecting nonlinearities can lead to rather severe errors in the overall solution. Currently we are testing a version of the HIGRAD code with the Newton-Krylov solver on simple fluid flow problems.

Computational Efficiency. The HIGRAD code has been adapted to run on LANL's ASCI parallel computing platform. Simulations have been run using upwards of 100 processors with turn-around times dropping from several weeks on typical workstations to a few hours on the ASCI machines. In addition, we are currently working on a compressible form of the HIGRAD model employing the method of averaging technique (MOA) to increase the efficiency of the code. The temporal averaging of sound waves allows for a time step very much larger than would be dictated by the speed of sound. Hence, model runtime will be reduced dramatically. The MOA approach also has the advantage of being potently more accurate than traditional implicit approaches.

Turbulence Parameterizations. Initial studies have begun on assessing the different types of large eddy simulation (LES) turbulence closures. Currently, the Smagorinsky and prognostic tke approaches are implemented into the HIGRAD code. The LES scheme allows for calculation of the fluctuating nature of the turbulent flow field. Although the LES scheme is computationally more expensive than the traditional Reynolds Averaged Navier Stokes (RANS) approaches, for some applications -- estimation of the peak concentration from a toxic agent release, for example – only the LES approach is appropriate. We are just now beginning validation of the LES schemes through comparison to turbulence measurements made in the EPA meteorological wind tunnel.

Future Outlook: Two extremely important tasks have begun recently and will be major focus areas for CFD model development in the near term. The first is validation using the high fidelity mean and turbulence flow measurements being obtained around building arrays at the USEPA meteorological wind tunnel. These datasets are critical for the evaluation of the assumptions found in the CFD codes (e.g., turbulence closures, boundary conditions, numerical schemes). The second is the rather laborious task of introducing grid nesting into HIGRAD. For the chem-bio project, HIGRAD is being tasked to run at scales from 10-100's of meters over a domain size in which the horizontal extent can be as large as 100 km. A domain of this size using 10 m resolution would call for 100,000+ nodal points, which even today is too large for parallel computations. To circumvent this problem we are introducing grid nesting into HIGRAD. Nesting will enable the code to be run at high resolution in the vicinity of the domain used by building-scale models and lower resolution elsewhere. The lower resolution domain of HIGRAD will be designed to match the highest resolution domain of the mesoscale model, e.g., COAMPS, providing a reasonable transition from the meso- to microscale.

References

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